

NEW RESULTS ON EIGENVALUES AND DEGREE DEVIATION

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ABSTRACT. Let G be a graph. In a famous paper Collatz and Sinogowith had proposed to measure its deviation from regularity by the difference of the (adjacency) spectral radius and the average degree: $\epsilon(G) = \rho(G) - \frac{2m}{n}$.

We obtain here a new upper bound on $\epsilon(G)$ which seems to consistently outperform the best known upper bound to date, due to Nikiforov. The method of proof may also be of independent interest, as we use notions from numerical analysis to re-cast the estimation of $\epsilon(G)$ as a special case of the estimation of the difference between Rayleigh quotients of proximal vectors.

1. INTRODUCTION AND MAIN RESULT

Let G be a connected graph with adjacency matrix A . Then A has a Perron value ρ and a positive Perron unit vector v that satisfy

$$Av = \rho v, \|v\|_2 = 1.$$

Suppose that the graph G has n vertices and m edges. Then $\frac{2m}{n}$ is equal to the average vertex degree of G . The following classic result of Collatz and Sinogowitz relates it to the Perron value:

Theorem 1.1. [6] *Let G be a connected graph with n vertices and m edges. Then*

$$(1) \quad \rho \geq \frac{2m}{n}$$

and equality holds if and only if G is regular.

Theorem 1.1 allows us to consider $\epsilon(G) = \rho - \frac{2m}{n}$ as a measure of the graph's irregularity. As such it has been studied by various authors

Date: February 11, 2013.

1991 *Mathematics Subject Classification.* 05C50, 05C07, 15A42, 91D30.

Key words and phrases. irregularity, adjacency matrix, Perron vector, Perron value, mean degree, harmonic graph, spectral radius, Rayleigh quotient numerical analysis.

This research was supported by the Israel Science Foundation (grant number 862/10.)

[1, 2, 5, 13, 15]. For some alternative ways of measuring the irregularity see [8]. We also call attention to [14] where (1) is placed in a wider context.

The inspiration for the present paper is given by the results of Nikiforov [13] who related $\epsilon(G)$ to two other natural measures of irregularity which are based on the degree sequence of G . These are in fact the first two moments of the degree sequence:

$$s(G) = \sum_{u \in V(G)} \left| d_u - \frac{2m}{n} \right|$$

and

$$\text{var}(G) = \frac{1}{n} \sum_{u \in V(G)} \left(d_u - \frac{2m}{n} \right)^2,$$

where d_u is the degree of the vertex u .

As observed in [13], $s(G)$ and $\text{var}(G)$ are related:

$$\frac{s^2(G)}{n^2} \leq \text{var}(G) \leq s(G).$$

Another interesting property of $\text{var}(G)$ can be obtained from the Popoviciu inequality [17]:

$$\text{var}(G) \leq \frac{(\Delta(G) - \delta(G))^2}{4}.$$

Our goal is to improve on the following result of Nikiforov:

Theorem 1.2. [13] *Let G be a graph. Then*

$$(2) \quad \frac{\text{var}(G)}{2\sqrt{2m}} \leq \epsilon(G) \leq \sqrt{s(G)}.$$

Let $S = \|v\|_1$, that is the sum of the entries of the unit Perron eigenvector. Note that by Cauchy-Schwarz, $S^2 \leq n$, with equality iff the graph G is regular, and thus S^{-1} may also serve as a measure of irregularity.

Theorem 1.3. *Let G be a connected graph. Then*

$$(3) \quad \epsilon(G) \leq \sqrt{\text{var}(G)} \cdot \sqrt{\frac{n}{S^2} - 1}.$$

The proof requires a brief detour into the field of numerical analysis, taking [19, Section 2] as our benevolent guide. Let M be a real symmetric matrix and $x \neq 0$ a (real) vector. The *Rayleigh quotient* is

$$\varrho(x) = \frac{x^T M x}{x^T x}.$$

It is well-known that the eigenvalues of M are precisely the stationary points of $\varrho(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}$.

Suppose now that $Ax = \lambda x$, so that $\varrho(x) = \lambda$. Suppose also that y is a vector lying close to x . We can expect by the continuity of $\varrho(\cdot)$ that $\varrho(x)$ will be close to $\varrho(y)$. Since the function $\varrho(\cdot)$ is homogenous, the useful way to measure proximity of vectors will be by the angle between x and y :

$$\angle(x, y) = \arccos \frac{|\langle x, y \rangle|}{\|x\|_2 \cdot \|y\|_2}.$$

There are two ways of making this statement precise: the *a priori* bound (4) and the *a posteriori* bound (5). The latter bound uses the residual vector $r(y) = Ay - \varrho(y)y$.

$$(4) \quad |\lambda - \varrho(y)| \leq (\lambda_{\max}(M) - \lambda_{\min}(M)) \cdot \sin^2(\angle(x, y)).$$

$$(5) \quad |\lambda - \varrho(y)| \leq \frac{\|r(y)\|}{\|y\|} \cdot \tan(\angle(x, y)).$$

It is not possible to tell in advance which of the bounds will turn out more useful for a particular problem. For our purposes the *a posteriori* works much better, so we will henceforth focus on it.

Let us take $M = A$ and $x = v$ and $y = \mathbf{1}_n$. Then we have that $\lambda = \rho(G)$ and $\varrho(y) = \frac{2m}{n}$. The residual vector $r(y)$ is:

$$r(y) = Ay - \varrho(y)y = d - \frac{2m}{n}.$$

Therefore

$$(6) \quad \frac{\|r(y)\|}{\|y\|} = \sqrt{\text{var}(G)}.$$

On the other hand, the cosine of the angle between v and $\mathbf{1}_n$ is:

$$(7) \quad \cos \angle(v, \mathbf{1}_n) = \frac{|\langle v, \mathbf{1}_n \rangle|}{\|v\|_2 \cdot \|\mathbf{1}_n\|_2} = \frac{S}{\sqrt{n}}.$$

The claim of Theorem 1.3 now follows from (5, 6, 7). □

Remark 1.4. *Extensive numerical calculations indicate that the bound of (3) is stunningly close to the true value of $\epsilon(G)$ in all cases examined. However, the actual estimation of S^2 on which the bound depends is often very difficult. Therefore, we are willing to settle for a weaker bound: $\epsilon(G) \leq \sqrt{\text{var}(G)}$ which would still improve upon Theorem 1.2. This fails to be true for disconnected graphs but we strongly believe that it is true for connected graphs.*

Conjecture 1.5. *If G is connected, then*

$$\epsilon(G) \leq \sqrt{\text{var}(G)}.$$

Clearly, the conjecture is equivalent to

$$S^2 \geq \frac{n}{2}.$$

2. FIRST EXAMPLES - EXACT COMPUTATION OF S^2

In order to demonstrate the strength of Theorem 1.3 we would like to consider first a number of examples in which the Perron vector v can be easily computed explicitly, and therefore a formula for S^2 can be written down.

Later we will develop some ways of estimating S^2 from below in cases where explicit expressions for v are not available or are too intimidating to be effectively used.

2.1. Bicliques. Let $G = K_{p,q}$ be a complete bipartite graph, with $p \leq q$. It is not hard to compute that $\rho(G) = \sqrt{pq}$ and

$$\epsilon(G) = \sqrt{pq} - \frac{2pq}{q+p}.$$

Nikiforov's estimate is:

$$\epsilon(G) \leq \sqrt{s(G)} = \sqrt{2pq \frac{(q-p)}{q+p}},$$

which has the correct order of magnitude but is off by multiplicative and additive constants. Let us now compute the bound of Theorem 1.3:

$$\sqrt{\text{var}(G)} = \frac{(q-p)}{q+p} \sqrt{pq},$$

and the Perron vector of

$$A(G) = \begin{bmatrix} J_p & 0 \\ 0 & J_q \end{bmatrix}$$

is easily verified to be

$$v = \begin{bmatrix} \frac{1}{\sqrt{2q}} \cdot \vec{j}_p \\ \frac{1}{\sqrt{2p}} \cdot \vec{j}_q \end{bmatrix}.$$

Therefore $S = \frac{1}{\sqrt{2}}(\sqrt{q} + \sqrt{p})$ and

$$\sqrt{\frac{n}{S^2} - 1} = \frac{\sqrt{q} - \sqrt{p}}{\sqrt{q} + \sqrt{p}}.$$

Finally, a simple algebraic manipulation will show that in this case equality obtains in (3) and thus our bound is sharp.

2.2. Harmonic graphs. A graph is called *harmonic* [7, 10] if for some real λ the equality $\lambda d_{v_i} = \sum_{j \sim i} d_{v_j}$ holds for all $i = 1, 2, \dots, n$. This is clearly equivalent to

$$\rho = \lambda, \quad v = c \cdot d, c > 0.$$

In this case we can evaluate the term S precisely.

Let us define the quantity

$$Z_G = \sum_{v \in V(G)} d_v^2$$

(cf. e.g. [16, 11]). Then

$$(8) \quad v = \sqrt{Z_G} \cdot d$$

for a harmonic graph.

Theorem 2.1. *Let G be a harmonic graph on n vertices and with m edges. Then*

$$(9) \quad \epsilon(G) \leq \sqrt{\text{var}(G)} \cdot \sqrt{\frac{nZ_G}{4m^2} - 1}.$$

Proof. By (8) we have

$$S^2 = \frac{4m^2}{Z_G}.$$

□

Example 2.2. *Consider a family of 3-harmonic graphs, constructed in [3]. See Figure 1. The graph T_k has $n = 3k$ vertices and $m = 4k$ edges. It has k vertices of degree 4 and $2k$ vertices of degree 2, therefore $\frac{2m}{n} = \frac{8}{3}$ and $\epsilon(G) = \frac{1}{3}$.*

Nikiforov's estimate (2) gives:

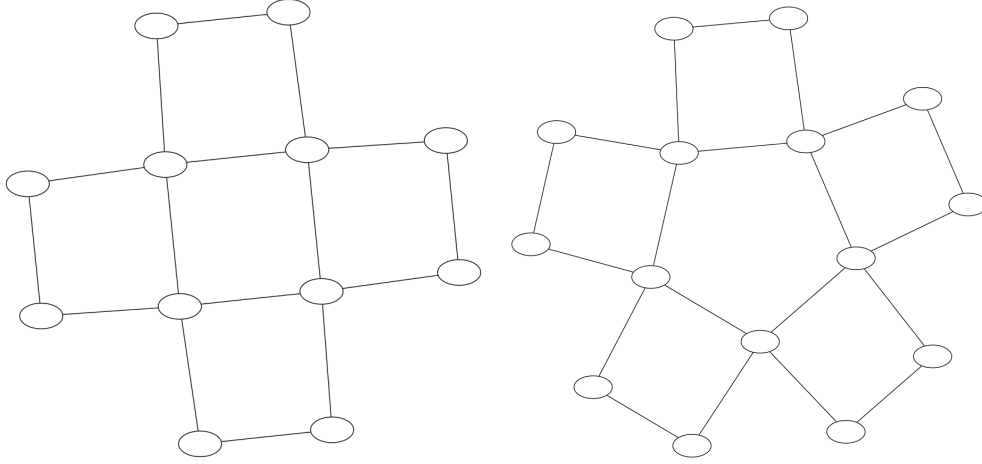
$$\epsilon(G) \leq \sqrt{s(G)} = \sqrt{\frac{8k}{3}},$$

failing to flesh out the fact that $\epsilon(G)$ is constant for the whole family.

On the other hand, $Z_G = 24k$ and $\text{var}(G) = \frac{8}{9}$ and thus from (9):

$$\epsilon(G) \leq \sqrt{\text{var}(G)} \cdot \sqrt{\frac{nZ_G}{4m^2} - 1} = \sqrt{\frac{1}{8}} \cdot \sqrt{\frac{8}{9}} = \frac{1}{3}.$$

So once again, equality holds.

FIGURE 1. T_4 and T_5

3. ESTIMATING S^2 BY THE WILF METHOD

Recall the classic result due to Wilf:

Theorem 3.1. [18] *Let G be a graph with clique number ω and spectral radius ρ . Then*

$$(10) \quad S^2 \geq \frac{\omega}{\omega - 1} \rho.$$

Wilf's result is in many cases sufficiently powerful to obtain, in conjunction with Theorem 1.3, excellent estimates on $\epsilon(G)$. In particular we can use it to prove our Conjecture 1.5 in a special case:

Corollary 3.2. *If G is a connected graph on n vertices with $\omega(G) \geq \frac{n}{2}$, then*

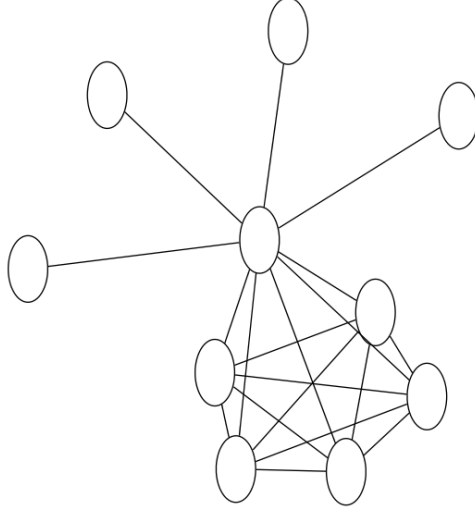
$$\epsilon(G) \leq \sqrt{\text{var}(G)}.$$

Proof. Since the spectral radius is monotone with respect to subgraphs (cf. [4, p. 33]) we have $\rho \geq \omega - 1$. Therefore $S^2 \geq \omega \geq \frac{n}{2}$. \square

In the remainder of this section we will study a particular example.

3.1. Pineapples. The pineapple graph $P(n, q)$ consists of a clique on q vertices and a stable set on $n - q$ vertices, so that one particular vertex in the clique is adjacent to all the vertices in the stable set. Pineapple graphs have high values of $\epsilon(G)$ and in fact have been conjectured to be its maximizers:

Conjecture 3.3. [1] *Among all graphs on $n \geq 10$ vertices the graph G with the highest value of $\epsilon(G)$ is $G = PA(n, q)$, $q = \lfloor \frac{n}{2} \rfloor + 1$.*

FIGURE 2. The graph $P(10, 6)$

Example 3.4. Consider the graph $G = P(2k, k + 1)$. Nikiforov's estimate is:

$$\epsilon(G) \leq \sqrt{s(G)} = \sqrt{\frac{k^3 - 3k + 2}{k}}.$$

Since $\omega = k + 1 \geq k = \frac{n}{2}$ we can use Corollary 3.2 to obtain:

$$\epsilon(G) \leq \sqrt{\text{var}(G)} = \frac{k-1}{2k} \cdot \sqrt{k^2 + 4k - 4}.$$

Thus an improvement by a factor of two is gained.

4. ESTIMATING S^2 FOR CONES

Let us now consider the case when $\Delta(G) = n - 1$, *i.e.* when some vertex is adjacent to all other vertices. Such a vertex is called *dominating* or *universal*. Denote by H the subgraph obtained by deleting v and all edges incident upon it from G . Another common mode of speaking is to say that G is the *cone* over H and the notation $G = H \vee K_1$ is used accordingly.

The pineapple graph is in fact a cone over the disjoint union of a clique and a stable set. As we have seen, for the pineapple graph the Wilf method works very well.

However, in other cases, it may yield poor results. Therefore we shall now develop an alternative method of estimating S^2 specifically for cones and then illustrate its power by an example.

Theorem 4.1. [9] *Let G be a connected graph on vertices $\{1, 2, \dots, n\}$ with Perron vector v , normalized so that $\|v\|_2 = 1$. For every vertex $i \in V(G)$ let $H_i = G - \{i\}$ be the subgraph obtained by deleting i from G and let ρ_{H_i} be its spectral radius. Then for any $1 \leq i \leq n$:*

$$(11) \quad v_i^2 \geq \frac{1}{1 + \frac{d_i}{(\rho - \rho_{H_i})^2}}.$$

Lemma 4.2. *Let G be a graph with vertex set $\{1, 2, \dots, n\}$ and suppose that 1 is a dominating vertex. Then*

$$(12) \quad S = (\rho + 1)v_1.$$

Proof. Consider the first entries of both sides of the equation $Av = \rho v$:

$$\rho v_1 = (Av)_1 = \sum_{j=2}^n v_j = S - v_1$$

□

Now, combining (11) and (12) we immediately obtain:

Theorem 4.3. *Let $G = H \vee K_1$ and let ρ_H be the spectral radius of H . If G has n vertices, then:*

$$(13) \quad S^2 \geq \frac{(\rho + 1)^2(\rho - \rho_H)^2}{(\rho - \rho_H)^2 + n - 1}.$$

Note that the right-hand side of (13) is a decreasing function of $\rho - \rho_H$ and therefore we can estimate it from below, in turn, by using bounds of the form $\rho \geq a$ and $\rho_H \leq b$, to obtain:

$$S^2 \geq \frac{(a + 1)^2(a - b)^2}{(a - b)^2 + n - 1}.$$

Example 4.4. *Let $G = P_{20} \vee K_1$ be the cone over the path on 20 vertices. To fairly compare the bounds on S^2 provided by (10) and (13) we will use Hofmeister's [12] bound $\rho \geq \sqrt{\frac{1}{n} \sum_{i=1}^n d_i^2}$ for both. Since the degrees of G are: $n - 1$, 3 repeated $n - 3$ times, and 2 repeated twice, we have:*

$$\rho \geq \sqrt{\frac{1}{n}(n^2 + 7n - 18)} = 5.21.$$

Thus, (10) yields:

$$S^2 \geq \frac{3}{2}\rho \geq 7.815,$$

whereas (13) yields, using $\rho_H \leq \Delta(H) = 2$:

$$S^2 \geq 13.115.$$

The actual value of S^2 in this example is 16.8305 while the right-hand side of (13) is 16.5815.

5. ACKNOWLEDGMENTS

I wish to thank Dr. Clive Elphick for illuminating correspondences on the subject of this paper and Professor Martin Golumbic for a careful reading of a first draft.

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